Thiane, 2-butyl

Other names: 2-Butylthiane
Inchi: InChI=1S/C9H18S/c1-2-3-6-9-7-4-5-8-10-9/h9H,2-8H2,1H3
InchiKey: SFIKCPNNQVZUDI-UHFFFAOYSA-N
Formula: C9H18S
SMILES: CCCCC1CCCCS1
Mol. weight [g/mol]: 158.30

Physical Properties

Property code	Value	Unit	Source
gf	89.21	kJ/mol	Joback Method
hf	-129.51	kJ/mol	Joback Method
hfus	14.56	kJ/mol	Joback Method
hvap	41.87	kJ/mol	Joback Method
log10ws	-3.48		Crippen Method
logp	3.462		Crippen Method
mcvol	143.160	ml/mol	McGowan Method
pc	2820.33	kPa	Joback Method
rinpol	1212.00		NIST Webbook
rinpol	1212.00		NIST Webbook
tb	472.70	K	Joback Method
tc	686.14	K	Joback Method
tf	282.02	K	Joback Method
vc	0.518	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.13	J/mol×K	472.70	Joback Method
cpg	325.74	J/mol×K	508.27	Joback Method
cpg	343.36	J/mol×K	543.85	Joback Method
cpg	360.02	J/mol×K	579.42	Joback Method
cpg	375.75	J/mol×K	614.99	Joback Method
cpg	390.58	J/mol×K	650.56	Joback Method
cpg	404.55	J/mol×K	686.14	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R41673&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume